5-Methyluridine, tris(trifluoroacetate)

Inchi: InChI=1S/C16H11F9N2O9/c1-4-2-27(13(32)26-8(4)28)9-7(36-12(31)16(23,24)25)6(35-1
InchiKey: FDCYXEIHTGKUSP-UHFFFAOYSA-N
Formula: C16H11F9N2O9
SMILES: Cc1cn(C2OC(COC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C2OC(=O)C(F)(F)F)c(=O)[nH]c1=O
Mol. weight [g/mol]: 546.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.39		Crippen Method
logp	0.314		Crippen Method
mcvol	277.500	ml/mol	McGowan Method
rinpol	1964.10		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U380304&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices